Phosphorodichloridothioic acid, O-methyl ester

Other names: Dichloromethoxyphosphine sulfide
Methyl dichlorothionophosphate
Methyl dichlorothiophosphate
O-Methyl phosphorodichloridothioate
O-Methyl phosphorodichlorothioate
Phosphorodichloridothioic acid, methyl ester
O-Methyl dichlorothiophosphate
Methyldichlorthiofosfat
O-Methylester kyseliny dichlorthiofosforecne

Inchi: InChI=1S/CH3Cl2OPS/c1-4-5(2,3)6/h1H3

InchiKey: BJTWJPDCJVKDBK-UHFFFAOYSA-N

Formula: CH3Cl2OPS

SMILES: COP(=S)(Cl)Cl

Mol. weight [g/mol]: 164.98

CAS: 2523-94-6

Physical Properties

Property code	Value	Unit	Source
ie	9.85	eV	NIST Webbook
log10ws	2.11		Crippen Method
logp	2.335		Crippen Method
mcvol	92.110	ml/mol	McGowan Method

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C2523946&Units=SI

Legend

ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume